

=> b reg  
FILE 'REGISTRY' ENTERED AT 14:48:58 ON 17 AUG 2009  
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STRUCTURE FILE UPDATES: 16 AUG 2009 HIGHEST RN 1174375-84-8  
DICTIONARY FILE UPDATES: 16 AUG 2009 HIGHEST RN 1174375-84-8

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experimental property data in the original document. For information  
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<http://www.cas.org/support/stngen/stndoc/properties.html>

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GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 9  
STEREO ATTRIBUTES: NONE
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SEARCH TIME: 00.00.01

=> b zcap  
FILE 'ZCAPLUS' ENTERED AT 14:49:04 ON 17 AUG 2009  
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FILE COVERS 1907 - 17 Aug 2009 VOL 151 ISS 8

FILE LAST UPDATED: 16 Aug 2009 (20090816/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLus family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> d bib abs hitstr 117 tot

L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN  
 AN 2005:823712 ZCPLUS  
 DN 143:229891  
 TI Diazabicyclic aryl derivatives as nicotinic acetylcholine receptor ligands and their preparation and pharmaceutical compositions  
 IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Oestergaard; Jorgensen, Tino Dyring; Ahring, Philip K.; Timmermann, Daniel B.  
 PA Neurosearch A/S, Den.  
 SO PCT Int. Appl., 49 pp.  
 CODEN PIXXD2

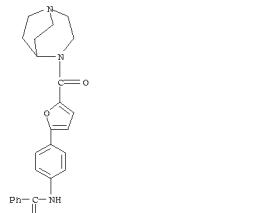
DT Patent  
 LA English  
 FAN,CNT 1

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2005WO-BP050405	W	20050201		
OS CASREACT 143:229891; MARPAT 143:229891				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to a group of diazabicyclic aryl derivs. I, including its enantiomers, N-oxides, prodrugs, and pharmaceutically acceptable salts, which are cholinergic ligands at the nicotinic acetylcholine receptors. In compd. I, n and X are 1 or 2 and are independently selected from (un)substituted aromatic monocyclic/polycyclic carbocycles/heterocycles; Z is an (un)substituted monocyclic heterocycle, amino, (thio)carboxyamino, imidamido, ureido, thioureido, or guanidino; and L is a bond, CH<sub>2</sub>, CH=CH<sub>2</sub>, CH-CH=C, C(=O)N, O, S, SCH<sub>2</sub>, etc. The invention also relates to the preparation of I, pharmaceutical compositions containing I or a pharmaceutically acceptable salt of I, the use of I as an lead one pharmaceutical acceptable carrier or diluent, as well as to the use of the compns. for the treatment of diseases and disorders associated with nicotinic acetylcholine receptors. 3-Quinuclidinone hydrochloride was condensed with 2-nitrobenzylamine and ring expansion followed by reduction with LiAlD<sub>4</sub> gave the formation of 2-(4-nitrophenyl)-3-quinuclidinone (III). III was acylated with 5-(4-nitrophenyl)-2-furyl chloride (preparation in situ from the corresponding acid is given) to give III. Palladium-catalyzed hydrogenation of III followed by addition to Et isocyanate gave diazabicyclic derivative IV. Compound IV expressed IC<sub>50</sub> value of 0.56 nM in a study on the

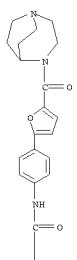
L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)  
 inhibition of [<sup>3</sup>H]-<sup>2</sup>-bungarotoxin in rat brain, representing the  $\alpha_7$ -subtype of nicotinic receptors.  
 IT 713599-85-6 (4-[5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)furan-2-yl)phenyl]benzamide **862851-89-6P**,  
 4-Amino-N-[4-(5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)furan-2-yl)phenyl]benzamide **862851-89-6P**,  
 3-Amino-N-[4-(5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)furan-2-yl)phenyl]benzamide **862851-29-7P**,  
 N-[4-(5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)furan-2-yl)phenyl]benzamide **862852-30-0P** **862852-33-3P**,  
 N-[4-((5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)furan-2-yl)phenyl)-2-nitrobenzamide **862852-43-5P**,  
 N-[4-((5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)furan-2-yl)phenyl)-2-nitrobenzamide **862852-44-6P**,  
 PL: PAC (Pharmacological activity); SPN (Synthetic preparation); IHS (Uses);  
 (Drug candidate); preparation of diazabicyclic aryl derivs. as nicotinic acetylcholine receptor ligands  
 RN 752499-87-5 ZCPLUS  
 CN Benzamide, N-(4-((5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)-2-furanyl)phenyl)- (CA INDEX NAME)



RN 862851-87-4 ZCPLUS  
 CN Benzamide, 4-amino-N-(4-((5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)-2-furanyl)phenyl)- (CA INDEX NAME)

L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)

PAGE 1-A



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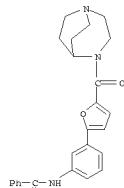


L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)

PAGE 2-A



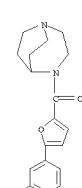
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RN 862852-30-0 ZCPLUS  
 CN Benzamide, N-(3-((5-((1,4-Diazabicyclo[3.2.2]non-4-yl)carbonyl)-2-furanyl)phenyl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

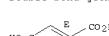
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CM 2

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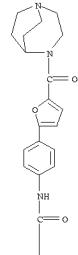
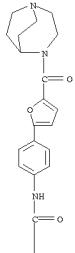
Double bond geometry as shown.



L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)

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CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-2-nitro-, hydrochloride (1:1) (CA INDEX NAME)

PAGE 1-A



PAGE 1-A

RN 862852-43-5 ZCPLUS  
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-2-nitro- (CA INDEX NAME)

● HCl



PAGE 2-A

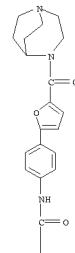
IT **862851-38-5P**, N-[4-[5-(1,4-Diazabicyclo[3.2.2]non-4-ylcarbonyl)furan-2-yl]phenyl]-4-nitrobenzamide **862851-90-9P**,  
N-[4-[5-(1,4-Diazabicyclo[3.2.2]non-4-ylcarbonyl)furan-2-yl]phenyl]-3-nitrobenzamide **862852-35-5P**,  
N-[4-[5-((1,4-Diazabicyclo[3.2.2]non-4-ylcarbonyl)furan-2-yl)phenyl]-4-nitrobenzamide hydrochloride **862852-37-7P**,  
N-[4-[5-((1,4-Diazabicyclo[3.2.2]non-4-ylcarbonyl)furan-2-yl)phenyl]-3-nitrobenzamide hydrochloride  
PL: RCT (Reactant); SPM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(Intermediate); preparation of diazabicyclic aryl derivs. as nicotinic acid/glycolic acid receptor ligands)

RN 862851-90-9 ZCPLUS  
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-4-nitro- (CA INDEX NAME)

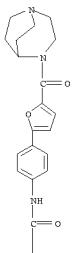
L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)

L17 ANSWER 1 OF 2 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)

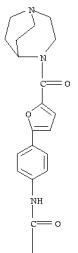
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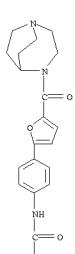
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RN 862851-90-9 ZCPLUS  
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-3-nitro- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RN 862851-90-9 ZCPLUS  
CN Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-3-nitro- (CA INDEX NAME)

● HCl

IT **862852-37-7** ZCPLUS  
Benzamide, N-[4-[5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl]phenyl]-3-nitro-, hydrochloride (1:1) (CA INDEX NAME)

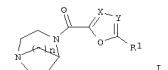


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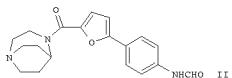
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L18 ANSWER 1 OF 1 ZCPLUS COPYRIGHT 2009 ACS on STN  
 AN 2004:740327 ZCPLUS  
 DN 141:260783  
 TI Preparation of diazabicyclic aryl derivatives as cholinergic ligands at the nicotinic acetylcholine receptors  
 IN Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Jorgensen, Tino Dyring; Ahring, Philip K.  
 PA Neurosearch A/S, Den.  
 SO PCT Int. Appl., 48 pp.  
 COOPER, PIXXD2  
 DT Patent  
 LA English  
 FAN,CNT 1

PATENT NO. KING DATE APPLICATION NO. DATE  
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 LK, LR, LS, LY, LV, MA, MD, MG, MN, MR, MT, NC, ND, NE,  
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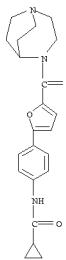


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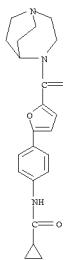
AB Title compds. represented by the formula I (wherein X, Y = independently CR2, CR3, N; R1 = H, (cyclo)alkyl, halo, etc.; R2, R3 = independently H, (cyclo)alkyl, alkyl, nitro, aryl, etc.; n = 1-3; and their enantiomers, any mixture of enantiomers, a prodrug, or pharmaceutically acceptable salts thereof) were prepared as cholinergic ligands at the nicotinic acetylcholine receptors.

L18 ANSWER 1 OF 1 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)



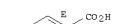
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CM 1  
 CRN 753499-91-1  
 CMF C22 H25 N3 O3



CM 2  
 CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



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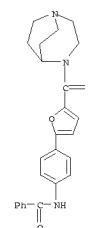
L18 ANSWER 1 OF 1 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)  
 receptors. For example, reaction of (1,4-diazabicyclo[3.2.2]non-4-yl)-5-(4-aminophenyl)furan-2-ylmethanone and EG-foamate yields in 53% yield. IC<sub>50</sub> value is 0.17 μM. Thus, I and their pharmaceutical compns. are useful as cholinergic ligands at the nicotinic acetylcholine receptors for the treatment of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction,ocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chem. substances (no data).

IT 753499-98-6P 753499-91-1P 753499-92-2P  
 PU: PAC (Pharmacological activity); SP: (Synthetic preparation); THU (Therapeutic use); BIDL (Biological study); PREP (Preparation); USES (Uses);

RN 753499-98-6 ZCPLUS  
 CN Benzamide, N-(4-(5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl)phenyl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 753499-97-5  
 CMF C25 H25 N3 O3



CM 2  
 CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 753499-91-1 ZCPLUS  
 CN Cyclopropanecarboxamide, N-[4-(5-(1,4-diazabicyclo[3.2.2]non-4-ylcarbonyl)-2-furanyl)phenyl]- (CA INDEX NAME)

L18 ANSWER 1 OF 1 ZCPLUS COPYRIGHT 2009 ACS on STN (Continued)  
 RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'REGISTRY' ENTERED AT 14:30:24 ON 17 AUG 2009  
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L4 46 L3 AND NC5-NC2NC3/ES AND OC4/ES

L5 STR

L6 225 (NC5-NC2NC3 AND OC4)/ES

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L8 14 L5 FULL SUB=L6  
SAV TEM J749C1G2/A L8

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L10 3 L8 NOT L9

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L12 4 L11 AND L6

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L14 1 L12 NOT L13

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L16 3 L10,L14

FILE 'ZCAPLUS' ENTERED AT 14:47:41 ON 17 AUG 2009

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